

Anisotropic spin and charge transport in Rashba Hamiltonian.

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Abstract

We explore spin and charge transport phenomena in two dimensional electron gas in presence of Rashba spin-orbit coupling connected to two ideal Ferromagnetic leads. In particular we show through a combination of analytical and numerical calculation that the spin polarization which is transported depends on the Magnetization direction of ferromagnet even if the magnetization of both FM's are parallel. Conductance is also shown to be anisotropic. These anisotropies present in spin and charge transport are a consequence of breaking of rotational invariance due to Rashba spin-orbit interaction and are present irrespective of the Hamiltonian considered being an effective mass Hamiltonian or tight binding model Hamiltonian.

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The growing field of spintronics has attracted a lot of interest after the proposal of spin-filed effect transistor (SPIN-FET) by Datta and Das [1]. The Datta-Das SPIN-FET is a hybrid structure of type FM1-2DEG-FM2, where 2DEG is a two-dimensional electron gas of a narrow gap semiconductor (InAs) and FM1 and FM2 are injector and detector Ferromagnetic contacts. The working of this device relies on the manipulation of electronic spin state in 2DEG with the electric field of an external gate electrode. Essential for this mechanism is field dependent spin-orbit coupling, which is relatively large and well established [2]. It is now generally accepted that the spin-orbit coupling in narrow-gap 2DEG is governed by Rashba Hamiltonian [3]. For a 2DEG lying in xy plane (see Fig.1) the Rashba spin-orbit interaction has the form, $H_R = \alpha(\mathbf{k} \times \sigma) \cdot \hat{z}$, with \mathbf{k} being momentum vector, σ

Pauli matrices and \hat{z} is a unit vector perpendicular to 2DEG plane. The Rashba spin-orbit causes spin splitting for $\mathbf{k} \neq 0$, $\Delta E = 2\alpha k$, which is linear in momentum. The Rashba splitting is due to lack of space inversion symmetry and not due to lack of time reversal symmetry. Since Rashba Hamiltonian is time reversal invariant. However the exchange splitting in Ferromagnets is due to the breaking of time reversal symmetry. Therefore it is natural to expect that spin and charge transport properties of a hybrid structure like SPIN-FET, which combines elements with different symmetry properties, may be different than the standard mesoscopic structures consisting of elements with same symmetry, for, e.g., all metal mesoscopic structures.

Motivated by this, in this paper we study the spin and charge transport of a FM1-2DEG-FM2 system shown in FIG. 1. The question we are addressing is the following: Consider the Fig.1, a natural reference frame for the Fig.1 is defined by the plane of 2DEG (we call it xy plane) and the normal to this plane, i.e., the z axis. The polarization of the Ferromagnets FM1 and FM2 are parallel to each other and points in a direction (θ, ϕ) with respect to the natural coordinate system *i.e.* make an angle θ with z axis and an angle ϕ with the x axis. Now the question is does the spin polarization which is transported from FM1 to FM2 and the charge transport, i.e, conductance depends on (θ, ϕ) ? In other words if we rotate the polarization vector of Ferromagnets simultaneously with respect to the natural coordinate system in such a way that they always remains parallel, does conductance and spin polarization which is transported changes? Naively speaking one would expect that the conductance and transported spin-polarization should be independent of (θ, ϕ) as long as both the Ferromagnets are parallel. In contrast to naive expectation we show through a combination of analytical and numerical calculation that spin polarization which is transported and charge conductance are anisotropic and these anisotropies are present irrespective of the Hamiltonian considered being an effective mass Hamiltonian [4] or tight binding Hamiltonian [5]. In this sense this is a rather general principal which says the polarization of transported electron across a FM/2DEG/FM2 and conductance is anisotropic and is a consequence of breaking of rotational invariance due to spin-orbit coupling. This is

in contrast to the claim made by Molenkamp et. al. [4] that the effective mass Hamiltonian does not have conductance anisotropy while the tight binding model [5] has due to reduced symmetry of lattice. Another important consequence of our study is it points out that spin coherence is also anisotropic, *i.e.* it depends on the chosen basis.

The Hamiltonian of a 2DEG lying in xy plane (as shown in Fig. 1), in presence of Rashba spin-orbit coupling reads: [3]

$$H = -\frac{\hbar \nabla^2}{2m} + \alpha(\sigma \times \mathbf{k}) \cdot \hat{\mathbf{z}} \quad (1)$$

where α Rashba spin-orbit interaction parameter and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices and $\hat{\mathbf{z}}$ is unit vector along the z axis. We write the above Hamiltonian in the matrix form which is more convenient for the study of spin transport

$$H = \frac{1}{2}(B_0 \mathbf{I} + \mathbf{B}_R \cdot \sigma) \quad (2)$$

where \mathbf{I} is the 2×2 identity matrix, $B_0 = \frac{\hbar^2(k_x^2 + k_y^2)}{2m}$ and the vector is $\mathbf{B}_R = 2\alpha(k_y \hat{\mathbf{x}} - k_x \hat{\mathbf{y}})$.

An appropriate physical quantity to study the spin transport is the Polarization vector $\mathbf{P} = \langle \sigma \rangle$ where angular brackets represents the ensemble averaging. With this definition one can immediately write down the equation of motion for polarization vector,

$$\begin{aligned} \frac{d\mathbf{P}}{dt} &= \frac{d\langle \sigma \rangle}{dt} = -\frac{i}{\hbar} \langle \sigma H - H \sigma \rangle \\ &= \frac{1}{2i\hbar} \langle \sigma (\mathbf{B}_R \cdot \sigma) - (\mathbf{B}_R \cdot \sigma) \sigma \rangle \end{aligned} \quad (3)$$

simplifying above equation using vector identities for triple product and commutation relation for Pauli matrices leads to following equation of motion for polarization vector,

$$\frac{d\mathbf{P}}{dt} = \mathbf{B}_R \times \langle \sigma \rangle. \quad (4)$$

The eq. (4) is well known in the literature and is a fully quantum mechanical and holds even if \mathbf{B}_R is time dependent. The eq. (4) can be solved analytically when the field \mathbf{B}_R is a constant vector, the most general solution is given as;

$$\begin{aligned} \mathbf{P}(t) = & \mathbf{P}_0 \cos(\omega_R t) + 2\hat{\mathbf{B}}_{\mathbf{R}}(\hat{\mathbf{B}}_{\mathbf{R}} \cdot \hat{\mathbf{P}}_0) \sin^2(\omega_R t/2) \\ & + (\hat{\mathbf{B}}_{\mathbf{R}} \times \hat{\mathbf{P}}_0) \sin(\omega_R t) \end{aligned} \quad (5)$$

where \mathbf{P}_0 is the initial polarization imposed by Ferromagnet FM1 (we are interested in the case when the Polarization of both the Ferromagnets FM1 and FM2 are parallel and equal in magnitude, *i.e.*, $\mathbf{P}_1 = \mathbf{P}_2 = \mathbf{P}_0$), $\omega_R = B_R/\hbar$ is precession frequency (precession angle $\phi = \omega_R t$), $B_R = 2\alpha\sqrt{k_x^2 + k_y^2}$ is the magnitude of Rashba field $\mathbf{B}_{\mathbf{R}}$ (the direction of $\mathbf{B}_{\mathbf{R}}$ is always perpendicular to the instantaneous wave vector \mathbf{k}). During electrons free flight the direction and magnitude of $\mathbf{B}_{\mathbf{R}}$ remains constant hence the solution provided by eq.(5) is applicable only during the free flight. Since scattering from impurity or boundary changes the momentum and hence the field $\mathbf{B}_{\mathbf{R}}$, so the time occurring in eq.(5) is free flight time. However for the ballistic transport we will use the eq.(5) and take into account the boundary scattering later in diffusive approximation as we will see later. Now since we are interested in the transport properties when the polarization of both the Ferromagnets are parallel to each other but pointing in arbitrary direction (θ, ϕ) such that $\mathbf{P}_1 = \mathbf{P}_2 = \mathbf{P}_0 = P_0(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ such that with respect to hence by projecting $\mathbf{P}(t)$ on \mathbf{P}_0 we get the,

$$\mathbf{P}(t) \cdot \mathbf{P}_0 = |\mathbf{P}_0|^2 \cos(\omega_R t) + (\mathbf{P}_0 \cdot \hat{\mathbf{B}}_{\mathbf{R}})^2 \sin^2(\omega_R t/2), \quad (6)$$

where $\omega_R = B_R/\hbar \equiv 2\alpha k_f/\hbar$. The eq.(6) is the quantitative measure of spin polarization which gets transported through the 2DEG from FM1 to FM2. For a given injection angle β as shown in Fig. 1, the eq.(6) simplifies to,

$$\begin{aligned} Pol(\theta, \phi, L, W, \omega_R t) & \equiv \frac{\mathbf{P}(t) \cdot \mathbf{P}_0}{|\mathbf{P}_0|^2} \\ & = \cos(\omega_R t) + \sin(\beta - \phi)^2 \sin^2(\theta)^2 \sin^2(\omega_R t/2) \end{aligned} \quad (7)$$

In the above equation t is the time electron takes to reach the output terminal and it is clear from eq.(7) that value of transported polarization, *i.e.*, $Pol(\theta, \phi, L, W, \omega_R t)$, lies between +1 and -1. Since the electron are injected over $-\pi/2 \leq \beta \leq \pi/2$, we need to make an average

over all possible values of injection angle β . However depending upon injection angle β electron reaches the boundary without scattering(dashed trajectory in Fig. 1) or with scattering (solid trajectory in Fig.1) from the boundaries. Hence we need to calculate t accordingly for different values of β . Therefore we divide the integration over β in three regimes, namely, (a) $-\pi/2 \leq \beta \leq -\tan^{-1}(W/2L)$, (b) $-\tan^{-1}(W/2L) \leq \beta \leq \tan^{-1}(W/2L)$ and (c) $\tan^{-1}(W/2L) \leq \beta \leq \pi/2$ where (a) and (c) corresponds to the trajectories which suffers scattering from boundary while trajectories in regime (b) propagates ballistically. For injection angle β in the regime (b) electron reaches the output terminal(FM2) ballistically therefore the time to reach the output terminal is $t = L/\cos(\beta)$ (see Fig.1 dashed line), while for regime (b) and (c) electron scatters from the boundary at least once before reaching the output terminal(FM2), hence for these values of β we assume that the electrons diffuse along the channel with a mean free path $W/2 \sin(\beta)$ (later in our exact numerical simulation we will see that this approximation is quite reasonable) so the time to reach the boundary is given as $t = (2L^2 \sin(\beta))/(v_f W)$. Using these value for t we get

$$\omega_R t = \begin{cases} \frac{2\alpha k_f L}{v_f \cos(\beta)} \equiv \frac{2\pi\tilde{\alpha}\tilde{L}}{\cos(\beta)} & \beta \in \{-\tan^{-1}(\frac{W}{2L}), \tan^{-1}(\frac{W}{2L})\} \\ \frac{2\alpha k_f L^2 \sin(\beta)}{v_f W} \equiv \frac{4\pi\tilde{\alpha}\tilde{L}^2 \sin(\beta)}{\tilde{W}} & \beta \in \{\pm\frac{\pi}{2}, \pm\tan^{-1}(\frac{W}{2L})\} \end{cases} \quad (8)$$

where $\tilde{\alpha} = \alpha k_f / E_f$ is dimensionless Rashba parameter(E_f is Fermi energy), $\tilde{L} = L/\lambda_f$ and $\tilde{W} = W/\lambda_f$ is length and width of channel in units of Fermi wavelength. Substituting these values of $\omega_R t$ in eq.(7) and performing the integration over β we obtain polarization as function of $\theta, \phi, \tilde{L}, \tilde{W}, \tilde{\alpha}$. Eq.(7) together with eq.(8) can be used to calculate the transported polarization for any given direction (θ, ϕ) , however for clarity and simplicity we present results for three specific cases corresponding to different values of θ and ϕ , namely, (i) $\theta=0$, ϕ is variable, i.e., polarization of FM1 nad FM2 is rotated in xy plane (the plane formed by 2DEG) (ii) $\phi=0$, θ is variable corresponding to the rotation in xz plane (iii) $\phi=\pi/2$, θ is variable, corresponding to the rotation in yz plane. For these three different cases the transported polarization given by eq.(7) is shown in Fig.2 as a function of angle , where the other parameters are $\tilde{L} = \tilde{W} = 50/(2\pi)$ and $\tilde{\alpha} = 0.06$. It is clearly seen from Fig.2 that

polarization which is transported is anisotropic, it is a consequence of spin-orbit coupling which breaks the rotational symmetry. The amplitude of oscillation tells about the spin coherence and since this is different for all the three cases, signifying that the spin coherence is also affected anisotropically. Infact it is seen from fig.2 that amplitude of oscillation is larger for the case (i) and (ii), when the polarization vector of Ferromagnets lies in yz or xy , compared to the case (iii). The absolute magnitude of oscillation is always smaller than one implying even in ballistic transport spin dephasing takes place due to the boundary scattering .

To further strengthen our results we performed numerical simulation on a tight binding square lattice of lattice spacing a with N_x sites along x axis and N_y sites along y axis. For tight binding Hamiltonian the Rashba spin-orbit coupling is given by $\lambda_{so} = \alpha/2a = \tilde{\alpha}tk_f a/2$. We fix $t=1$ (hopping) and $k_f a=1$ (ballistic case) for numerical simulation in tight binding model. Once t and $k_f a$ are fixed the other parameters for tight binding model which would corresponds to the parameters of Fig. 1 are given as, $N_x = 2\pi\tilde{L} = 50, N_y = 2\pi\tilde{W} = 50$ and $\lambda_{so} = \tilde{\alpha}tk_f a/2 = 0.03$. With these set of parameters we calculate spin resolved conductance for a given polarization direction (θ, ϕ) of Ferromagnets, within Landauer-Büttiker formalism [6,5,8]. Using the spin resolved conductance we define polarization as

$$P = \frac{G_{sc} - G_{sf}}{G_{sc} + G_{sf}}. \quad (9)$$

where G_{sc} and G_{sf} are spin-conserved and spin flip conductance respectively. The quantity P in eq.(9) corresponds to the quantity given in eq.(7) and also lies between +1 and -1. This is plotted in Fig. 4 , we see that the agreement between Fig.3, i.e, analytical calculation, and Fig. 4 is quite good. The slight quantitative mismatch is due to the fact that numerical simulation was done for hard wall confining potential in y direction which leads to specular reflection, while in analytical calculation scattering from the boundary was treated as diffusive. Therefore it is clear that the anisotropy in spin transport is present in continuum model (effective mass Hamiltonian) as well as in tight binding model and is not an effect of reduced symmetry of tight binding model, rather it is a consequence of breaking

of rotational invariance due to spin orbit coupling.

Now since conductance of FM/2DEG/FM, depends on the polarization of electrons reaching the output terminal, hence it is expected that conductance should also be anisotropic. This is clearly visible in Fig. 5 where we have plotted total conductance, *i.e.*, $G = G_{sc} + G_{sf}$ corresponding to the Fig. 4, as function of polarization angle. It should be noted that the conductance is symmetric with respect to angle θ or ϕ which is consistent with Büttiker symmetry relation for charge transport [8]. It is important to point out that in recent literature [9] an erroneous result was reported, where it was claimed that conductance of a FM/2DEG interface changes on flipping the magnetization of FM which is incorrect.

The results presented above were in ballistic regime. To verify that these results survives in diffusive case we show polarization and conductance in Fig. 5 and Fig. 6 respectively for diffusive case. We have taken Anderson model for disorder with width $3|t|$, corresponding to a mean free path of $l = 10a$. The other parameters are same as those for Fig. 3 and Fig. 4. It is clearly seen that the anisotropy survives even in diffusive case. This only strengthen our previous assertion that spin coherence is anisotropic. Also it is instructive to compare Fig. 3 for ballistic transport and Fig. 5 for diffusive transport. It is seen that the polarization which is transported is not affected much by the presence of disorder which is consistent with the Rashba spin-orbit interaction which is independent of disorder strength. However the magnitude of charge conductance is reduced drastically as seen from Fig. 4 and Fig. 6, though the qualitative behavior as function of angle remains unchanged. This clearly demonstrates that the conductance anisotropy exist and is consistent with the Büttiker symmetry relation. One important thing to be noticed is the amplitude of oscillation for ballistic case as well for diffusive case for both polarization and conductance remains almost unchanged since the Rashba coupling was kept fixed for all the figures. This clearly demonstrates that the anisotropy is a consequence of spin-orbit interaction and is not affected by disorder.

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FIGURE CAPTINOS

1Fig.1 A 2DEG connected to two ideal Ferromagnetic leads.

2Fig2. Polarization as a function of angle calculated using eq.(7) and eq.(8).Where $\tilde{L} = \tilde{W} = 50/2\pi, \tilde{\alpha} = 0.06$.

3Fig.3 Results of numerical simulation for polarization for ballistic system. The numerical simulation were performed on a 50×50 lattice within tight binding model. The tight binding Rashba parameter is given by $\lambda_{so} = \tilde{\alpha} t k_f a / 2 = 0.03$, FM exchange splitting is $\Delta / E_f = 0.5$ and $k_f a = 1$. These parameters were chosen in such a way that they correspond to the parameters of Fig. 1, as explained in text.

4Fig.4 The conductance as a function of angle. The parameters are same as in Fig.3

5 Fig. 5 Polarization as a function of angle for diffusive case. Here $k_f l = 10$, where l is mean free path. Configuration averaging was performed over 15 different configuration. The other parameters are same as in Fig. 3

6 Fig. 6 Conductance as function of angle corresponding to the Fig. 5. Here $k_f l = 10$, where l is mean free path. Configuration averaging was performed over 15 different configuration. The other parameters are same as in Fig. 3









